

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Caesium diuranium hexatelluride

Adel Mesbah and James A. Ibers*

Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208, USA

Correspondence e-mail: ibers@chem.northwestern.edu

Received 28 August 2012; accepted 7 September 2012

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{Te}-\text{Te}) = 0.001$ Å; disorder in main residue; R factor = 0.022; wR factor = 0.053; data-to-parameter ratio = 32.2.

Single crystals of CsU_2Te_6 were synthesized from the reaction of U, Te, and Cs_2Te_3 at 1273 K. CsU_2Te_6 crystallizes in the space group $Cmcm$ in the CsTh_2Te_6 structure type. The asymmetric unit comprises one U (site symmetry $m2m$), one Cs ($m2m$; half-occupancy) and two Te atoms ($m..$ and $m2m$). The structure of CsU_2Te_6 consists of infinite $[\text{U}_2\text{Te}_6]$ layers perpendicular to $[010]$ separated by Cs atoms. There are infinite Te—Te—Te linear chains along $[001]$.

Related literature

For related structures, see: Narducci & Ibers (1998); Chan *et al.* (2004); Bugaris *et al.* (2010); Choi *et al.* (1998); Cody & Ibers (1996); Mizoguchi *et al.* (2006); Tougait *et al.* (1997); Krönert & Plieth (1965); Wu *et al.* (1997). For synthetic details, see: Bugaris & Ibers (2008); Haneveld & Jellinek (1969). For standardization of structural data, see: Gelato & Parthé (1987).

Experimental

Crystal data

CsU_2Te_6	$V = 652.06$ (5) Å ³
$M_r = 1374.57$	$Z = 2$
Orthorhombic, $Cmcm$	Mo $K\alpha$ radiation
$a = 4.2129$ (2) Å	$\mu = 40.65$ mm ⁻¹
$b = 25.6317$ (11) Å	$T = 100$ K
$c = 6.0385$ (2) Å	$0.21 \times 0.03 \times 0.02$ mm

Data collection

Bruker APEXII CCD diffractometer	5645 measured reflections
Absorption correction: numerical face-indexed (SADABS; Sheldrick, 2008a)	611 independent reflections
$T_{\min} = 0.043$, $T_{\max} = 0.482$	574 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$	19 parameters
$wR(F^2) = 0.053$	$\Delta\rho_{\text{max}} = 3.89$ e Å ⁻³
$S = 1.22$	$\Delta\rho_{\text{min}} = -1.87$ e Å ⁻³
611 reflections	

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008b); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008b); molecular graphics: CrystalMaker (Palmer, 2009); software used to prepare material for publication: SHELXL97.

The research was kindly supported at Northwestern University by the US Department of Energy, Basic Energy Sciences, Chemical Sciences, Biosciences, and Geosciences Division and Division of Materials Science and Engineering Grant ER-15522. Use was made of the IMSERC X-ray Facility at Northwestern University, supported by the International Institute of Nanotechnology (IIN).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2209).

References

- Bruker (2009). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bugaris, D. E. & Ibers, J. A. (2008). *J. Solid State Chem.* **181**, 3189–3193.
- Bugaris, D. E., Wells, D. M., Yao, J., Skanthakumar, S., Haire, R. G., Soderholm, L. & Ibers, J. A. (2010). *Inorg. Chem.* **49**, 8381–8388.
- Chan, B. C., Hulvey, Z., Abney, K. D. & Dorhout, P. K. (2004). *Inorg. Chem.* **43**, 2453–2455.
- Choi, K.-S., Patschke, R., Billinge, S. J. L., Waner, M. J., Dantus, M. & Kanatzidis, M. G. (1998). *J. Am. Chem. Soc.* **120**, 10706–10714.
- Cody, J. A. & Ibers, J. A. (1996). *Inorg. Chem.* **35**, 3836–3838.
- Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
- Haneveld, A. J. K. & Jellinek, F. (1969). *J. Less Common Met.* **18**, 123–129.
- Krönert, W. & Plieth, K. (1965). *Z. Anorg. Allg. Chem.* **336**, 207–218.
- Mizoguchi, H., Gray, D., Huang, F. Q. & Ibers, J. A. (2006). *Inorg. Chem.* **45**, 3307–3311.
- Narducci, A. A. & Ibers, J. A. (1998). *Inorg. Chem.* **37**, 3798–3801.
- Palmer, D. (2009). CrystalMaker Software. CrystalMaker Software Ltd, Oxford, England.
- Sheldrick, G. M. (2008a). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008b). *Acta Cryst.* **A64**, 112–122.
- Tougait, O., Daoudi, A., Potel, M. & Noël, H. (1997). *Mater. Res. Bull.* **32**, 1239–1245.
- Wu, E. J., Pell, M. A. & Ibers, J. A. (1997). *J. Alloys Compd.* **255**, 106–109.

supplementary materials

Acta Cryst. (2012). E68, i76 [doi:10.1107/S1600536812038512]

Caesium diuranium hexatelluride**Adel Mesbah and James A. Ibers****Comment**

CsU₂Te₆ (Figure 1) belongs to the AAn₂Q₆ (A= K, Rb, Cs, or Tl; An = U, Th, or Np; Q = S, Se, or Te) family. Compounds in this family crystallize in two different structures types: CsTh₂Te₆ (Cody & Ibers, 1996) (space group *Cmcm*) and KTh₂Se₆ (Choi *et al.*, 1998; Wu *et al.*, 1997) (space group *Immm*). Both structure types have AnQ₃ layers intercalated with A atoms. The difference between the two structure types is that each successive AnQ₃ layer in the *Cmcm* structure type is shifted by $a/2$, whereas each successive AnQ₃ layer in the *Immm* structure type is shifted by $(a + b)/2$ (Mizoguchi *et al.*, 2006). The AnQ₃ layers are analogous to those in the structure of ZrSe₃ (Krönert & Plieth, 1965). The CsTh₂Te₆ structure type is adopted by KTh₂Te₆ (Wu *et al.*, 1997) and Tl_{1.12}UTe₆ (Tougait *et al.*, 1997). The KTh₂Se₆ structure type is adopted by RbTh₂Se₆ (Choi *et al.*, 1998), K_{0.91}U_{1.79}S₆ (Mizoguchi *et al.*, 2006), KU₂Se₆ (Chan *et al.*, 2004; Mizoguchi *et al.*, 2006), CsU₂Se₆ (Choi *et al.*, 1998), CsTh₂Se₆, Rb_{0.85}U_{1.74}S₆, RbU₂Se₆, Cs_{0.88}(La_{0.68}U_{1.32})Se₆, KNp₂Se₆, CsNp₂Se₆, and TlU₂Se₆ (Bugaris *et al.*, 2010). The structures of the two last compounds are modulated and were refined in $5a \times 5b \times 5c$ and $4a \times 4b$ superlattices, respectively.

Experimental

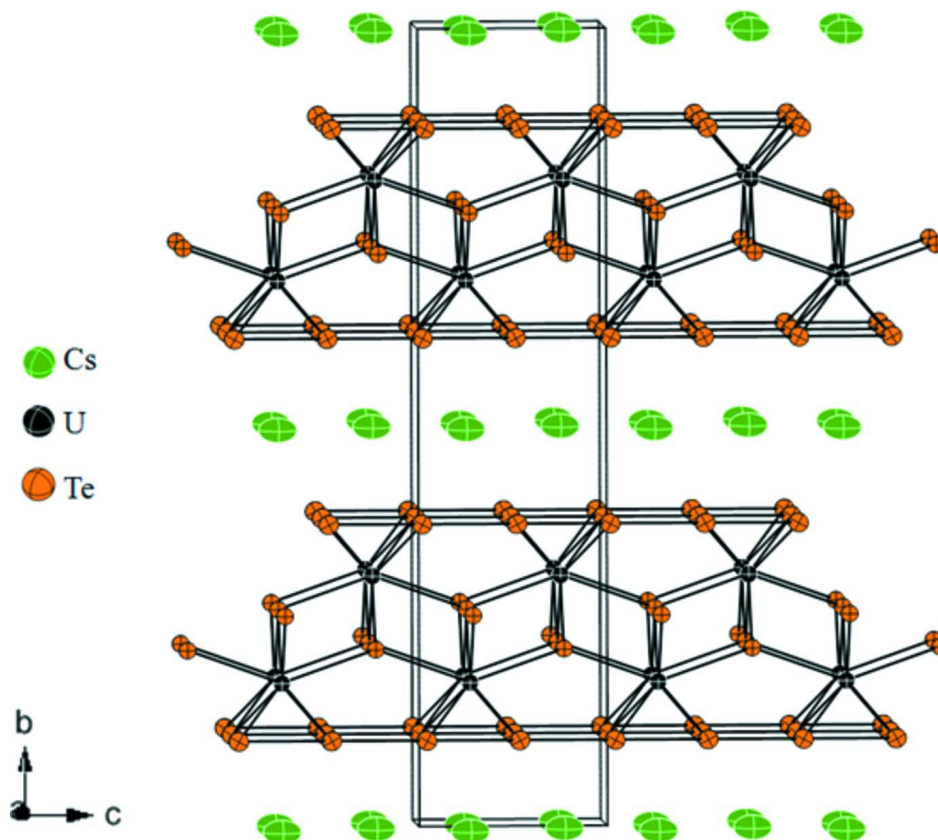
Black needles of CsU₂Te₆ were obtained by direct combination of ²³⁸U (30 mg, 12.9 mmol), Te (20.9 mg, 16.4 mmol, Aldrich, 99.8%) and Cs₂Te₃ (24.6 mg, 37.9 mmol). Cs₂Te₃ was prepared by the stoichiometric reaction of Cs (Alfa Aesar, 99.8%) and Te in liquid NH₃ at 194 K. U powder obtained by hydridization and decomposition of turnings (depleted, ORNL) by heating under vacuum, in a modification (Bugaris & Ibers, 2008) of a previous literature method (Haneveld & Jellinek, 1969). The starting reagents were loaded in a carbon-coated fused-silica tube under an Ar atmosphere in a glove box, then evacuated to 10⁻⁴ Torr, and flame sealed. The tube was placed in computer-controlled furnace, heated to 1273 K in 48 h, held there for 4 h, cooled to 1223 K in 12 h and kept there for 8 d, then cooled to 293 K at 3 K/h. Black needles were selected and analyzed by EDX and showed the formation of Cs:U:Te in a 1:2:6 ratio. The yield, based on U, was about 15% of the product.

Refinement

The highest peak (3.9 e⁻ Å⁻³) is 0.76 Å from atom Te1 and the deepest hole (1.9 e⁻ Å⁻³) is 0.78 Å from atom U1. These should be compared with the height of 225 e⁻ Å⁻³ of atom Te(1) in an electron density map.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008b); molecular graphics: *CrystalMaker* (Palmer, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008b).


Figure 1

Structure of CsU₂Te₆ viewed approximately down [100]. Displacement ellipsoids are drawn at the 95% probability level.

Caesium diuranium hexatelluride

Crystal data

CsU₂Te₆

$M_r = 1374.57$

Orthorhombic, *Cmcm*

Hall symbol: -C 2c 2

$a = 4.2129 (2) \text{ \AA}$

$b = 25.6317 (11) \text{ \AA}$

$c = 6.0385 (2) \text{ \AA}$

$V = 652.06 (5) \text{ \AA}^3$

$Z = 2$

$F(000) = 1102$

$D_x = 7.001 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2738 reflections

$\theta = 6.4\text{--}60.9^\circ$

$\mu = 40.65 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Needle, black

$0.21 \times 0.03 \times 0.02 \text{ mm}$

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: numerical

face-indexed (*SADABS*; Sheldrick, 2008a)

$T_{\min} = 0.043$, $T_{\max} = 0.482$

5645 measured reflections

611 independent reflections

574 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 30.7^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -5 \rightarrow 3$

$k = -36 \rightarrow 36$

$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.053$
 $S = 1.22$
 611 reflections
 19 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map
 $[1.00000]/[\sigma^2(F_o^2) + (0.0298F_o^2)^2]$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 3.89 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.87 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
U1	0.0000	0.685078 (14)	0.2500	0.00916 (11)	
Cs1	0.0000	0.49825 (7)	0.2500	0.0556 (7)	0.50
Te1	0.0000	0.116539 (18)	0.00249 (7)	0.01098 (13)	
Te2	0.0000	0.27322 (2)	0.2500	0.00877 (14)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.0072 (2)	0.01045 (17)	0.00982 (17)	0.000	0.000	0.000
Cs1	0.100 (2)	0.0194 (9)	0.0475 (12)	0.000	0.000	0.000
Te1	0.0087 (3)	0.0118 (2)	0.0125 (2)	0.000	0.000	-0.00052 (15)
Te2	0.0079 (3)	0.0090 (3)	0.0095 (3)	0.000	0.000	0.000

Geometric parameters (\AA , $^\circ$)

U1—Te2 ⁱ	3.0890 (5)	Cs1—Te1 ⁱⁱⁱ	3.9830 (15)
U1—Te2 ⁱⁱ	3.0890 (5)	Cs1—Te1 ⁱⁱ	3.9830 (15)
U1—Te1 ⁱⁱ	3.1237 (4)	Cs1—Cs1 ^{xi}	4.2129 (2)
U1—Te1 ⁱⁱⁱ	3.1237 (4)	Cs1—Cs1 ^{xii}	4.2129 (2)
U1—Te1 ^{iv}	3.1237 (4)	Te1—Te1 ^{xiii}	2.9892 (8)
U1—Te1 ⁱ	3.1237 (4)	Te1—Te1 ^{xiv}	3.0493 (8)
U1—Te2 ^v	3.2028 (3)	Te1—U1 ^{xv}	3.1237 (4)
U1—Te2 ^{vi}	3.2028 (3)	Te1—U1 ^{xvi}	3.1237 (4)
U1—Cs1	4.7888 (19)	Te1—Cs1 ^{vii}	3.9265 (14)
Cs1—Cs1 ^v	3.0206 (1)	Te1—Cs1 ^{ix}	3.9265 (14)
Cs1—Cs1 ^{vi}	3.0206 (1)	Te1—Cs1 ^{xvi}	3.9830 (15)
Cs1—Te1 ^{vii}	3.9266 (14)	Te1—Cs1 ^{xv}	3.9830 (15)
Cs1—Te1 ^{viii}	3.9266 (14)	Te2—U1 ^{xvi}	3.0889 (5)

Cs1—Te1 ^{ix}	3.9266 (14)	Te2—U1 ^{xv}	3.0889 (5)
Cs1—Te1 ^x	3.9266 (14)	Te2—U1 ^v	3.2028 (3)
Cs1—Te1 ^{iv}	3.9830 (15)	Te2—U1 ^{vi}	3.2028 (3)
Cs1—Te1 ⁱ	3.9830 (15)		
Te2 ⁱ —U1—Te2 ⁱⁱ	85.989 (18)	Te1 ^{ix} —Cs1—Te1 ⁱⁱⁱ	178.90 (3)
Te2 ⁱ —U1—Te1 ⁱⁱ	150.600 (9)	Te1 ^x —Cs1—Te1 ⁱⁱⁱ	135.105 (5)
Te2 ⁱⁱ —U1—Te1 ⁱⁱ	87.220 (10)	Te1 ^{iv} —Cs1—Te1 ⁱⁱⁱ	63.86 (3)
Te2 ⁱ —U1—Te1 ⁱⁱⁱ	150.600 (9)	Te1 ⁱ —Cs1—Te1 ⁱⁱⁱ	80.85 (4)
Te2 ⁱⁱ —U1—Te1 ⁱⁱⁱ	87.220 (10)	Cs1 ^v —Cs1—Te1 ⁱⁱ	110.64 (7)
Te1 ⁱⁱ —U1—Te1 ⁱⁱⁱ	57.172 (15)	Cs1 ^{vi} —Cs1—Te1 ⁱⁱ	66.56 (5)
Te2 ⁱ —U1—Te1 ^{iv}	87.220 (10)	Te1 ^{vii} —Cs1—Te1 ⁱⁱ	98.104 (9)
Te2 ⁱⁱ —U1—Te1 ^{iv}	150.600 (9)	Te1 ^{viii} —Cs1—Te1 ⁱⁱ	115.619 (7)
Te1 ⁱⁱ —U1—Te1 ^{iv}	111.555 (18)	Te1 ^{ix} —Cs1—Te1 ⁱⁱ	135.105 (5)
Te1 ⁱⁱⁱ —U1—Te1 ^{iv}	84.808 (13)	Te1 ^x —Cs1—Te1 ⁱⁱ	178.90 (3)
Te2 ⁱ —U1—Te1 ⁱ	87.220 (10)	Te1 ^{iv} —Cs1—Te1 ⁱⁱ	80.85 (4)
Te2 ⁱⁱ —U1—Te1 ⁱ	150.600 (9)	Te1 ⁱ —Cs1—Te1 ⁱⁱ	63.86 (3)
Te1 ⁱⁱ —U1—Te1 ⁱ	84.808 (13)	Te1 ⁱⁱⁱ —Cs1—Te1 ⁱⁱ	44.08 (2)
Te1 ⁱⁱⁱ —U1—Te1 ⁱ	111.555 (18)	Cs1 ^v —Cs1—Cs1 ^{xi}	90.0
Te1 ^{iv} —U1—Te1 ⁱ	57.172 (15)	Cs1 ^{vi} —Cs1—Cs1 ^{xi}	90.0
Te2 ⁱ —U1—Te2 ^v	75.873 (8)	Te1 ^{vii} —Cs1—Cs1 ^{xi}	57.556 (13)
Te2 ⁱⁱ —U1—Te2 ^v	75.873 (8)	Te1 ^{viii} —Cs1—Cs1 ^{xi}	57.556 (13)
Te1 ⁱⁱ —U1—Te2 ^v	129.697 (9)	Te1 ^{ix} —Cs1—Cs1 ^{xi}	122.442 (13)
Te1 ⁱⁱⁱ —U1—Te2 ^v	74.730 (11)	Te1 ^x —Cs1—Cs1 ^{xi}	122.442 (13)
Te1 ^{iv} —U1—Te2 ^v	74.730 (11)	Te1 ^{iv} —Cs1—Cs1 ^{xi}	121.930 (13)
Te1 ⁱ —U1—Te2 ^v	129.697 (9)	Te1 ⁱ —Cs1—Cs1 ^{xi}	121.930 (13)
Te2 ⁱ —U1—Te2 ^{vi}	75.873 (8)	Te1 ⁱⁱⁱ —Cs1—Cs1 ^{xi}	58.072 (13)
Te2 ⁱⁱ —U1—Te2 ^{vi}	75.873 (8)	Te1 ⁱⁱ —Cs1—Cs1 ^{xi}	58.072 (13)
Te1 ⁱⁱ —U1—Te2 ^{vi}	74.730 (11)	Cs1 ^v —Cs1—Cs1 ^{xii}	90.0
Te1 ⁱⁱⁱ —U1—Te2 ^{vi}	129.697 (9)	Cs1 ^{vi} —Cs1—Cs1 ^{xii}	90.0
Te1 ^{iv} —U1—Te2 ^{vi}	129.697 (9)	Te1 ^{vii} —Cs1—Cs1 ^{xii}	122.442 (13)
Te1 ⁱ —U1—Te2 ^{vi}	74.730 (11)	Te1 ^{viii} —Cs1—Cs1 ^{xii}	122.442 (13)
Te2 ^v —U1—Te2 ^{vi}	141.01 (2)	Te1 ^{ix} —Cs1—Cs1 ^{xii}	57.556 (13)
Te2 ⁱ —U1—Cs1	137.005 (9)	Te1 ^x —Cs1—Cs1 ^{xii}	57.556 (13)
Te2 ⁱⁱ —U1—Cs1	137.005 (9)	Te1 ^{iv} —Cs1—Cs1 ^{xii}	58.072 (13)
Te1 ⁱⁱ —U1—Cs1	55.777 (9)	Te1 ⁱ —Cs1—Cs1 ^{xii}	58.072 (13)
Te1 ⁱⁱⁱ —U1—Cs1	55.777 (9)	Te1 ⁱⁱⁱ —Cs1—Cs1 ^{xii}	121.930 (13)
Te1 ^{iv} —U1—Cs1	55.777 (9)	Te1 ⁱⁱ —Cs1—Cs1 ^{xii}	121.930 (13)
Te1 ⁱ —U1—Cs1	55.777 (9)	Cs1 ^{xi} —Cs1—Cs1 ^{xii}	180.0
Te2 ^v —U1—Cs1	109.494 (12)	Te1 ^{xiii} —Te1—Te1 ^{xiv}	180.00 (3)
Te2 ^{vi} —U1—Cs1	109.494 (12)	Te1 ^{xiii} —Te1—U1 ^{xv}	61.414 (8)
Cs1 ^v —Cs1—Cs1 ^{vi}	176.59 (14)	Te1 ^{xiv} —Te1—U1 ^{xv}	118.586 (8)
Cs1 ^v —Cs1—Te1 ^{vii}	114.23 (7)	Te1 ^{xiii} —Te1—U1 ^{xvi}	61.414 (8)
Cs1 ^{vi} —Cs1—Te1 ^{vii}	68.54 (5)	Te1 ^{xiv} —Te1—U1 ^{xvi}	118.586 (8)
Cs1 ^v —Cs1—Te1 ^{viii}	68.54 (5)	U1 ^{xv} —Te1—U1 ^{xvi}	84.806 (13)
Cs1 ^{vi} —Cs1—Te1 ^{viii}	114.23 (7)	Te1 ^{xiii} —Te1—Cs1 ^{vii}	112.848 (11)
Te1 ^{vii} —Cs1—Te1 ^{viii}	45.70 (2)	Te1 ^{xiv} —Te1—Cs1 ^{vii}	67.152 (11)
Cs1 ^v —Cs1—Te1 ^{ix}	114.23 (7)	U1 ^{xv} —Te1—Cs1 ^{vii}	165.69 (2)
Cs1 ^{vi} —Cs1—Te1 ^{ix}	68.54 (5)	U1 ^{xvi} —Te1—Cs1 ^{vii}	104.208 (12)

Te1 ^{vii} —Cs1—Te1 ^{ix}	64.89 (3)	Te1 ^{xiii} —Te1—Cs1 ^{ix}	112.848 (11)
Te1 ^{viii} —Cs1—Te1 ^{ix}	82.94 (4)	Te1 ^{xiv} —Te1—Cs1 ^{ix}	67.152 (11)
Cs1 ^v —Cs1—Te1 ^x	68.54 (5)	U1 ^{xv} —Te1—Cs1 ^{ix}	104.208 (12)
Cs1 ^{vi} —Cs1—Te1 ^x	114.23 (7)	U1 ^{xvi} —Te1—Cs1 ^{ix}	165.69 (2)
Te1 ^{vii} —Cs1—Te1 ^x	82.94 (4)	Cs1 ^{vii} —Te1—Cs1 ^{ix}	64.89 (3)
Te1 ^{viii} —Cs1—Te1 ^x	64.89 (3)	Te1 ^{xiii} —Te1—Cs1 ^{xvi}	67.961 (10)
Te1 ^{ix} —Cs1—Te1 ^x	45.70 (2)	Te1 ^{xiv} —Te1—Cs1 ^{xvi}	112.039 (10)
Cs1 ^v —Cs1—Te1 ^{iv}	66.56 (5)	U1 ^{xv} —Te1—Cs1 ^{xvi}	127.246 (13)
Cs1 ^{vi} —Cs1—Te1 ^{iv}	110.64 (7)	U1 ^{xvi} —Te1—Cs1 ^{xvi}	83.80 (2)
Te1 ^{vii} —Cs1—Te1 ^{iv}	178.90 (3)	Cs1 ^{vii} —Te1—Cs1 ^{xvi}	44.895 (5)
Te1 ^{viii} —Cs1—Te1 ^{iv}	135.105 (5)	Cs1 ^{ix} —Te1—Cs1 ^{xvi}	81.896 (9)
Te1 ^{ix} —Cs1—Te1 ^{iv}	115.619 (7)	Te1 ^{xiii} —Te1—Cs1 ^{xv}	67.961 (10)
Te1 ^x —Cs1—Te1 ^{iv}	98.104 (9)	Te1 ^{xiv} —Te1—Cs1 ^{xv}	112.039 (10)
Cs1 ^v —Cs1—Te1 ⁱ	110.64 (7)	U1 ^{xv} —Te1—Cs1 ^{xv}	83.80 (2)
Cs1 ^{vi} —Cs1—Te1 ⁱ	66.56 (5)	U1 ^{xvi} —Te1—Cs1 ^{xv}	127.246 (13)
Te1 ^{vii} —Cs1—Te1 ⁱ	135.105 (5)	Cs1 ^{vii} —Te1—Cs1 ^{xv}	81.896 (9)
Te1 ^{viii} —Cs1—Te1 ⁱ	178.90 (3)	Cs1 ^{ix} —Te1—Cs1 ^{xv}	44.895 (5)
Te1 ^{ix} —Cs1—Te1 ⁱ	98.104 (9)	Cs1 ^{xvi} —Te1—Cs1 ^{xv}	63.86 (3)
Te1 ^x —Cs1—Te1 ⁱ	115.619 (7)	U1 ^{xvi} —Te2—U1 ^{xv}	85.992 (18)
Te1 ^{iv} —Cs1—Te1 ⁱ	44.08 (2)	U1 ^{xvi} —Te2—U1 ^v	104.126 (8)
Cs1 ^v —Cs1—Te1 ⁱⁱⁱ	66.56 (5)	U1 ^{xv} —Te2—U1 ^v	104.126 (8)
Cs1 ^{vi} —Cs1—Te1 ⁱⁱⁱ	110.64 (7)	U1 ^{xvi} —Te2—U1 ^{vi}	104.126 (8)
Te1 ^{vii} —Cs1—Te1 ⁱⁱⁱ	115.619 (7)	U1 ^{xv} —Te2—U1 ^{vi}	104.126 (8)
Te1 ^{viii} —Cs1—Te1 ⁱⁱⁱ	98.104 (9)	U1 ^v —Te2—U1 ^{vi}	141.01 (2)

Symmetry codes: (i) $x+1/2, y+1/2, z$; (ii) $x-1/2, y+1/2, z$; (iii) $x-1/2, y+1/2, -z+1/2$; (iv) $x+1/2, y+1/2, -z+1/2$; (v) $-x, -y+1, -z+1$; (vi) $-x, -y+1, -z$; (vii) $-x-1/2, -y+1/2, -z$; (viii) $-x-1/2, -y+1/2, z+1/2$; (ix) $-x+1/2, -y+1/2, -z$; (x) $-x+1/2, -y+1/2, z+1/2$; (xi) $x-1, y, z$; (xii) $x+1, y, z$; (xiii) $x, y, -z+1/2$; (xiv) $x, y, -z-1/2$; (xv) $x+1/2, y-1/2, z$; (xvi) $x-1/2, y-1/2, z$.